

10/518,221

=> d his

(FILE 'HOME' ENTERED AT 00:39:24 ON 02 OCT 2006)

FILE 'REGISTRY' ENTERED AT 00:39:41 ON 02 OCT 2006

L1 SCREEN 964 AND 1006 AND 1051  
L2 STRUCTURE UPLOADED  
L3 QUE L2 AND L1  
L4 2 S L3 FUL

FILE 'CAPLUS' ENTERED AT 00:40:29 ON 02 OCT 2006

L5 13 S L4  
L6 2 S L4/P

FILE 'REGISTRY' ENTERED AT 00:41:51 ON 02 OCT 2006

L7 1 S ANILINE/CN

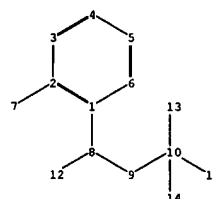
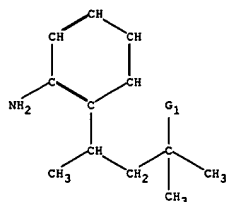
FILE 'CASREACT' ENTERED AT 00:47:05 ON 02 OCT 2006

L8 SCREEN 963 AND 970 AND 1006 AND 1015  
L9 STRUCTURE UPLOADED  
L10 QUE L9 AND L8  
L11 SCREEN 964 AND 970 AND 1006 AND 1015 AND 1051  
L12 STRUCTURE UPLOADED  
L13 QUE L12 AND L11

FILE 'CAPLUS' ENTERED AT 00:50:29 ON 02 OCT 2006

L14 11 S L5 NOT L6

=>



chain nodes :

7 8 9 10 11 12 13 14

ring nodes :

1 2 3 4 5 6

chain bonds :

1-8 2-7 8-9 8-12 9-10 10-11 10-13 10-14

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

2-7 10-13

exact bonds :

1-8 8-9 8-12 9-10 10-11 10-14

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

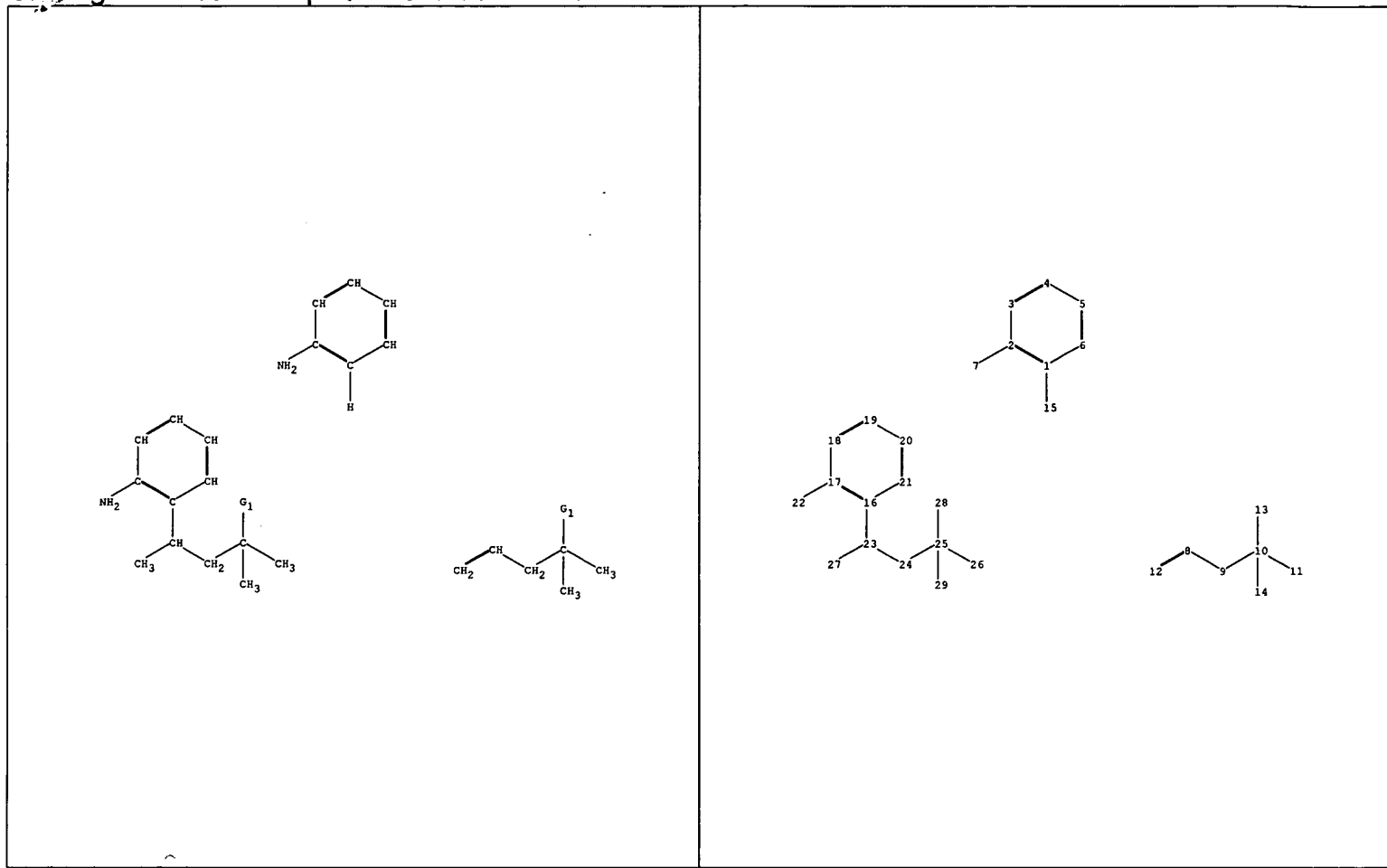
isolated ring systems :

containing 1 :

G1:H,CH3,Et

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS  
12:CLASS13:CLASS14:CLASS



chain nodes :

7 8 9 10 11 12 13 14 15 22 23 24 25 26 27 28 29

ring nodes :

1 2 3 4 5 6 16 17 18 19 20 21

chain bonds :

1-15 2-7 8-12 8-9 9-10 10-11 10-13 10-14 16-23 17-22 23-24 23-27 24-25 25-26 25-28 25-29

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

exact/norm bonds :

2-7 10-13 17-22 25-28

exact bonds :

1-15 8-12 8-9 9-10 10-11 10-14 16-23 23-24 23-27 24-25 25-26 25-29

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 16-17 16-21 17-18 18-19 19-20 20-21

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS8:CLASS9:CLASS10:CLASS11:CLASS  
12:CLASS13:CLASS14:CLASS15:CLASS16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:CLASS  
23:CLASS24:CLASS25:CLASS26:CLASS27:CLASS28:CLASS29:CLASS

fragments assigned reactant role:

containing 1  
containing 8

fragments assigned product role:

containing 16  
reaction site bonds:  
8-12:CC 1-15:CC